

Diatomic molecule as a quantum entanglement switch

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Abstract

We investigate a pair entanglement of electrons in diatomic molecule, modeled as a correlated double quantum dot attached to the leads. The low-temperature properties are derived from the ground state obtained by utilizing the Rejec-Ramšak variational technique within the framework of EDABI method, which combines exact diagonalization with *ab initio* calculations. The results show, that single-particle basis renormalization modifies the entanglement-switch effectiveness significantly. We also found the entanglement signature of a competition between an extended Kondo and singlet phases.

Key words: Correlated nanosystems, Entanglement manipulation, EDABI method
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Quantum entanglement, as one of the most intriguing features of quantum mechanics, have spurred a great deal of scientific activity during the last decade, mainly because it is regarded as a valuable resource in quantum communication and information processing [1]. The question on entanglement between microscopic degrees of freedom in a condensed phase have been raised recently [2], in hope to shed new lights on the physics of quantum phase transitions and quantum coherence [3]. In the field of quantum electronics, a pair entanglement appeared to be a convenient tool to characterize the nature of transport through quantum dot, since its vanish when the system is in a Kondo regime [4]. The analogical behavior was observed for two qubits in double quantum dot, for either *serial* and *parallel* configuration [5]. The latter case is intriguing, since the concurrence [6] at $T = 0$ changes abruptly from $\mathcal{C} \approx 1$ to $\mathcal{C} = 0$ when varying the interdot coupling, so a finite Anderson system shows a true quantum phase transition.

Here we consider a nanoscale version of such an *entanglement switch*, inspired by conductance measurements for a single hydrogen molecule [7]. A special attention is payed to electron-correlation effects, in particular the wave-function renormalization [8]. Recent experiment [9] shows the current through a molecule is carried by a single conductance channel, so serial configuration shown in Fig. 1 seems to be the realistic one. The Hamiltonian of the system is

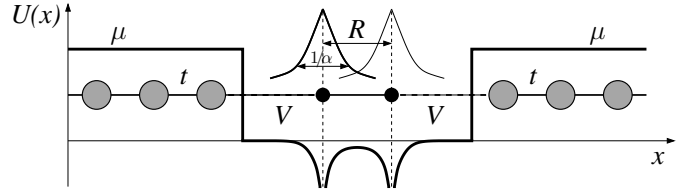


Fig. 1. Diatomic molecule modeled as a double quantum dot attached serially to the leads. A cross-section of the single-particle potential along the main system axis is shown schematically.

$$H = H_L + V_L + H_C + V_R + H_R, \quad (1)$$

where H_C models the central region, $H_{L(R)}$ describes the left (right) lead, and $V_{L(R)}$ is the coupling between the lead and the central region. Both $H_{L(R)}$ and $V_{L(R)}$ terms have a tight-binding form, with the chemical potential in leads μ , the hopping t , and the tunneling amplitude V , as depicted schematically in Fig. 1. The central-region Hamiltonian

$$H_C = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma \neq j\sigma'} U_{ij} n_{i\sigma} n_{j\sigma'} + (Ze)^2/R \quad (2)$$

(with $i, j = 1, 2$ and $\sigma = \uparrow, \downarrow$) describes a double quantum dot with electron-electron interaction. t_{ij} and U_{ij} are single-particle and interaction elements, the last term describes the Coulomb repulsion of the two ions at the distance R . Here we put $Z = 1$ and calculate all the parameters t_{ij} , U_{ij} as the Slater integrals [10] for 1s-like hydrogenic orbitals $\Psi_{1s}(\mathbf{r}) = \sqrt{\alpha^3/\pi} \exp(-\alpha|\mathbf{r}|)$, where α^{-1} is the orbital size (*cf.* Fig. 1). The parameter α is optimized to get a minimal ground-state energy for whole the system

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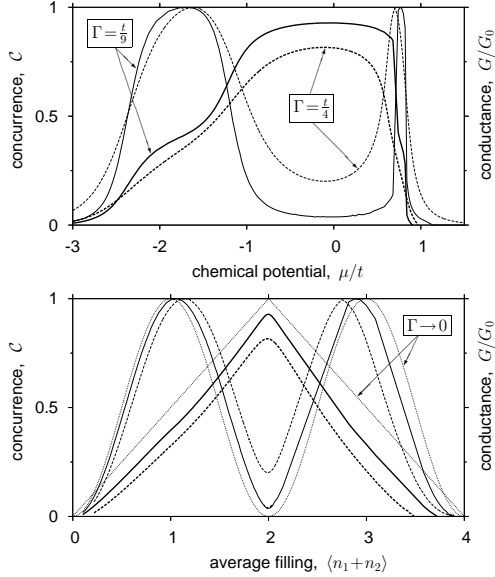


Fig. 2. Entanglement and transport through the system in Fig. 1 as a function of the chemical potential μ (*top panel*) and the average filling $\langle n_1 + n_2 \rangle$ (*bottom panel*). Tick (thin) *solid* and *dashed* lines shows the concurrence \mathcal{C} (conductance G) for $\Gamma = t/9$ and $t/4$, respectively. The limits $\Gamma \rightarrow 0$ are depicted with dotted lines in the bottom panel. The interatomic distance is $R = 1.5a_0$.

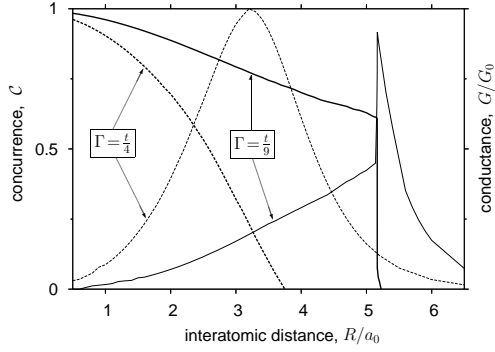


Fig. 3. Concurrence (*tick* lines) and conductance (*thin* lines) at the half-filled sector $\langle n_1 + n_2 \rangle = 2$ as a function of the interatomic distance R . The remaining parameters are the same as in Fig. 2.

described by the Hamiltonian (1). Thus, following the idea of EDABI method [8], we reduce the number of physical parameters of the problem to just a three: the interatomic distance R , the lead-molecule hybridization $\Gamma = V^2/t$, and the chemical potential μ (we put the lead hopping $t = 1 \text{ Ry} = 13.6 \text{ eV}$ to work in the wide-bandwidth limit).

The entanglement between electrons placed on two atoms can be characterized by the charge concurrence [4]

$$\mathcal{C} = 2 \max \left\{ 0, |\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle| - \sqrt{\langle n_{i\sigma} n_{j\sigma} \rangle \langle \bar{n}_{i\sigma} \bar{n}_{j\sigma} \rangle} \right\} \quad (3)$$

where $\bar{n}_{i\sigma} \equiv 1 - n_{i\sigma}$. We also discuss the conductivity calculated from the formula $G = G_0 \sin^2(E_+ - E_-)/4tN$ [11], where $G_0 = 2e^2/\hbar$, and E_\pm are the ground-state energies of the system with periodic and antiperiodic boundary conditions, respectively. Either the energies E_\pm or correla-

tion functions in Eq. (3) are calculated within the Rejec-Ramšak variational method [11], complemented by the orbital size optimization, as mentioned above. We use up to $N = 10^4$ sites to reach the convergence.

In Fig. 2 we show the concurrence and conductance for $R = 1.5a_0$ (where a_0 is the Bohr radius) and two values of the hybridization $\Gamma = t/9$ and $t/4$. The conductance spectrum asymmetry, caused by wave-function renormalization [8], is followed by an analogical effect on entanglement, which changes significantly faster for the upper conduction band, where the average filling is $\langle n_1 + n_2 \rangle \approx 3$ (one *extra electron*). The asymmetry vanishes when analyzing the system properties as a function of $\langle n_1 + n_2 \rangle$, showing it originates from varying charge compressibility $\chi_c = \partial \langle n_1 + n_2 \rangle / \partial \mu \approx 2/(U_{11} + U_{12}) \sim 1/\alpha$. We also note the convergence of discussed quantities with $\Gamma \rightarrow 0$ to $\mathcal{C} \approx 1 - |\langle n_1 + n_2 \rangle - 2|/2$ and $G \approx G_0 \sin^2(\pi \langle n_1 + n_2 \rangle / 2)$.

Entanglement evolution with R is illustrated in Fig. 3, where we focus on the charge neutral section $\langle n_1 + n_2 \rangle = 2$. The abrupt entanglement drop follows the sharp conductance peak for $\Gamma = t/9$, which is associated with the competition between double Kondo and spin/charge singlet phases [12]. For $\Gamma = t/4$ both \mathcal{C} and G dependence on R become smooth, but the switching behavior is still present. Earlier, we have shown that $\Gamma = t/4$ is large enough to cause molecule instability and therefore may allow the individual atom manipulation [8].

In conclusion, we analyzed a pair entanglement of electrons in diatomic molecule attached serially to the leads. Entanglement evolution with the chemical potential speeds up remarkably for the negatively charged system, due to electron correlation effects. The switching behavior was also observed when changing the interatomic distance.

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